Indian J. Phys. **78(10)**, 1079-1083 (2004)

IJP
INTERNATIONAL JOURNAL

Angular distribution for the proton impact ionization of $3p$-electrons in Ar

S Bhattacharya[1], K B Choudhury[2], N C Deb[3] and K Roy[3]*
[1]Department of Physics, Surendranath College, Kolkata-700 009, India
[2]Department of Physics, Charu Chandra College, Kolkata-700 029, India
[3]Department of Theoretical Physics, Indian Association for the Cultivation of Science, Kolkata-700 032, India

E-mail : tpkr@mahendra.iacs.res.in

Abstract : Using our recently published theoretical model for proton impact ionization of Ar [*Phys Rev*. **A68** 052702 (2003)], we calculate here the double differential cross sections for the same system at various ejected electron energies and angle of ejection. Results are compared with available measurements and other calculated results. It is found that our results agree reasonably well with the measurement in the binary encounter region but slightly overestimate the measurement around the recoil peak. At 350 keV impact energy we have calculated double differential cross sections for outgoing electron energies at (a) 46 eV, (b) 100 eV and (c) 308 eV. All three cases exhibit similar behaviour.

Keywords : Heavy particle impact ionization, differential cross section.

PACS Nos. : 34.50.Fa, 34.70.+e

1. Introduction

Ionization of atoms by heavy particle impact have received much attention to theoreticians as well as to the experimentalists due to many interesting behaviour in the angular and energy distribution of the ejected electrons. In the energy distribution of ejected electrons, when outgoing electron velocity matches with the projectile velocity, a sharp peak appears and it is known as the electron capture to the continuum (ECC) peak. Since it's discovery in 1970 the ECC peak [1] was known to occur at zero degree electrons and at equal velocity of the projectile and the ejected electron. Both of these characteristics have now been changed because of two recent measurements [2,3] and thereby generated new interest within the atomic physics community. Sarkadi *et al* [2] showed for the proton-impact ionization of Ar that ECC cusp do occur for non-zero degree electrons. On the other hand, Shah and coworkers [3] reported an ECC peak at an electron velocity slightly less than the projectile velocity in 10 keV and 20 keV proton on helium and hydrogen molecule. In the angular distributions of the outgoing electron, two peaks are expected to appear : one is called the binary encounter peak and the other is known as recoil peak. These double differential cross sections give far more insight than the corresponding total ionization cross sections. For example, the differential cross section allows us to study the dynamics of a free electron in the field of two Coulomb potentials.

In the present calculation, we shall concentrate on the angular distributions of the ejected electron with different momenta at a fixed projectile energy. Measurement of these angular distributions were carried out by Sarkadi *et al* [4] and Rudd *et al* [5]. On the theoretical side Fainstein *et al* [6] and Gulyás *et al* [7] reported results of angular distributions for proton impact ionization of Ar using continuum-distorted-wave eikonal initial state (CDW-EIS) approximation developed by Crothers and McCann [8]. The CDW-EIS results of Fainstein *et al* [6] show very good agreement with the measurement of Rudd *et al* [5]. However, experimental values at forward (below 20°) and backward (above 140°) angles are not available. Theoretical results for these angular regions show large disagreement among the various calculations and motivated us to study the angular distributions for

*Corresponding Author

proton impact ionization of Ar. In a recent calculation Bhattacharya *et al* [9] have resolved the low energy discrepancy for the total ionization cross sections of Ar by proton impact. Here, we apply their model to calculate the double differential cross sections as a function of the ejection angle of the ionized electron. In what follows, the description of the theoretical model used in the calculation.

2. Theory

In the present investigation, we have employed our recently published theoretical model to investigate the double differential cross sections for proton impact ionization of $3p$-electrons in Ar. Details of the theoretical model are given by Bhattacharya *et al* [9] and only a brief description is presented here. However, the evaluation of the transition matrix element is rather tricky and will be presented here in greater details in the next section. For the present model it is assumed that the interaction between the active electron and the residual ion is given by

$$V_A = -\frac{1}{r_A}\left[q_A + e^{-\lambda r_A}\{(Z-q_A)+br_A\}\right]$$

where q_A is the asymptotic charge of the residual target ion, Z is the nuclear charge of the target and r_A is the distance of the active electron from the nucleus of the same. The parameters b and λ are determined variationally with respect to the Slater basis set.

Following Bhattacharya *et al* [9], the transition amplitude can be expressed as

$$T_{fi}(p) = \iint\left[\Psi_{kc}^{-*}\left(H_{el} - i\frac{d}{dt}\right)\Psi_i^+\right]drdt, \tag{1}$$

where the Born initial state is given by

$$\Psi_i^+ = \sum_j C_j^{nl}\exp(-\beta_j r_A) r_A^l Y_{lm}(\hat{r}_A)\times e^{-\frac{i}{2}v.r}\times e^{-\left(i\varepsilon + \frac{i}{8}v^2\right)t}$$

which is an eigen state of

$$\left(-\frac{1}{2}\nabla_r^2 + V_A(r_A) - i\frac{\partial}{\partial t}\right).$$

Here, $\boldsymbol{r_A}$ and $\boldsymbol{r}$ are the position vectors of the active electron with respect to the target nucleus and the mid-point of two nuclei respectively. ε represents the eigen energy of the active electron in a state having the quantum numbers n, l, m; v is the velocity of the projectile with respect to the target.

The corresponding Hamiltonian in the final channel is given by

$$H_{el} = -\frac{1}{2}\nabla_r^2 + V_A(r_A) + V_B(r_B),$$

where r_B refers to the distance of the electron from the projectile and the associated wave function takes the form

$$\Psi_{kc}^- = (2\pi)^{-1.5}N_1N_2e^{ik.r}\,{}_1F_1(i\alpha_B,1;-i(k_Br_B+\boldsymbol{k}_B.\boldsymbol{r}_B))$$
$$\times{}_1F_1(i\alpha_A,1;-i(k_Ar_A+\boldsymbol{k}_A.\boldsymbol{r}_A))e^{-ik^2t/2},$$

where $\alpha_B = -\frac{Z_B}{\,}$, $\alpha_A = -\frac{q_A}{\,}$, $\boldsymbol{k}_B = \boldsymbol{k} - \frac{\boldsymbol{v}}{\,}$, $\boldsymbol{k}_A = \boldsymbol{k} +$

and

$$N_1 = e^{-\pi\alpha_B/2}\Gamma(1+i\alpha_B),\quad N_2 = e^{-\pi\alpha_A/2}\Gamma(1+i\alpha_A)$$

with Z_B as the nuclear charge of the projectile and q_A as the asymptotic charge of the target ion. While deriving eq. (1), we have used the impact parameter formalism and treated the inter-nuclear separation classically through $\boldsymbol{R} = \boldsymbol{p} + \boldsymbol{v}t$, with p being the impact parameter. Here, the time has been measured from the instant when the two nuclei are at their closest approach. Obviously, the initial condition is given by the fact that $T_{fi}(p)$ tends to zero as t equals to negative infinity and the probability ionization is $|T_{fi}(t=+\infty)|^2$.

The double differential cross sections are then expressed as

$$\frac{d^2\sigma}{dE_e d\Omega_e} = k\iint|T_{fi}(p)|^2dp. \tag{2}$$

2.1. Evaluation of $T_{fi}(p)$:

In order to evaluate the transition matrix element, we have placed the centre of our reference frame at the mid-point of the two nuclei. This choice gave us some advantage to evaluate some of the integrals analytically. It is to be noted here that the final state wave function in the present model differs from the corresponding wave functions used in the CDW-EIS model, which resulted from the different choice of coordinate system. The transition matrix element can be expressed as

$$T_{fi}(p) = -N_1^*N_2^*(I_1+I_2), \tag{3}$$

where

$$I_1 = \int {}_1g_1 \times \tau(t) \times g_k dr dt \sum_{j=1}^{L} C_j r_A e^{-\lambda_j r_A} \cos\theta_A$$

and

$$I_2 = \int {}_1g_1 \times \tau(t) \times g_k dr dt \sum C_j r_A^2 e^{-\lambda_j r_A} \cos\theta_A$$

with

$${}_1g_1 = e^{-ik.r}\,{}_1F_1\left(-i\alpha_B,1;i(k_B r_B + \boldsymbol{k}_B \boldsymbol{r}_B)\right)$$

$$\times {}_1F_1\left(-i\alpha_A,1;i(k_A r_A + \boldsymbol{k}_A \boldsymbol{r}_A)\right),$$

$$\tau(t) = \frac{e^{ik^2 t/2}}{r_B}$$

and

$$g_k = e^{-i\frac{v^2 t}{8} - i\varepsilon t - \frac{i}{2}v.r}.$$

I_1 and I_2 can be readily evaluated by noting that we have two integrals of the form :

$$J_1 = \int g_k \tau(t)\,{}_1g_1 r_A e^{-\lambda r_A} \cos\theta_A dr dt$$

and

$$J_2 = \int g_k \tau(t)\,{}_1g_1 r_A^2 e^{-\lambda r_A} \cos\theta_A dr dt$$

which can be evaluated by considering a single integral of the form,

$$J = \int {}_1g_1 \times g_k \frac{e^{i\frac{k^2 t}{2}} e^{-\lambda r_A} e^{-\mu r_B}}{r_A r_B} e^{i\delta . r_A} dr dt, \text{ with } \mu \to 0$$

and $\delta \to 0$, such that J_1 and J_2 can be generated from J in the following manner :

$$J_1 = -\frac{1}{i}\frac{\partial^2 J}{\partial\delta_z \partial\lambda}\bigg|_{\mu\to 0,\,\delta\to 0} \text{ and } J_2 = \frac{1}{i}\frac{\partial^3 J}{\partial\delta_z \partial^2\lambda}\bigg|_{\mu\to 0\,\delta\to 0}. \tag{4}$$

In evaluating J, use has been made of the Fourier transform technique and the contour integral representation of the confluent hypergeometric functions contained in ${}_1g_1$ and thus we obtain,

$$J = -\frac{1}{4\pi^2}\int e^{iEt} dt \oint t_1^{-i\alpha_B - 1}(t_1 - 1)^{i\alpha_B} dt_1 \times$$
$$\oint t_2^{-i\alpha_A - 1}(t_2 - 1)^{i\alpha_A} dt_2 \times J' dt,$$

such that

$$J' = \int e^{ik\,r} \exp\left(i(k_B r_B + \boldsymbol{k}_B \boldsymbol{r}_B)t_1\right) \times \exp\left(i(k_A r_A + \boldsymbol{k}_A \boldsymbol{r}_A)t_2\right)$$
$$\times \frac{e^{-\lambda r_A - \mu r_B} e^{i\delta . r_A}}{r_B r_A} dr$$

with $E = \frac{k^2}{2} - \frac{v^2}{8} - \varepsilon$ and $K = k + v/2$, and finally J' reduces to

$$J' = \frac{2}{\pi}\int \frac{e^{iQ.R}}{(A - Bt_1)(C - Dt_2)} dQ$$

with $A = (Q - K/2)^2$, $B = -2\boldsymbol{k}_B.(Q - K/2)$,

$$C = (Q + K/2)^2 + \lambda^2,$$

and $D = 2i\lambda k_A + 2\boldsymbol{k}_A.(Q + K/2)$, with $\mu \to 0$, $\delta \to 0$.

If the Z-axis is chosen along the direction of $\boldsymbol{v}$, the three dimensional vectors $\boldsymbol{Q}$ and $\boldsymbol{K}$ can be represented in the following manner : $\boldsymbol{Q} = \boldsymbol{Q}_z + \boldsymbol{p}$ and $\boldsymbol{K} = \boldsymbol{k}_z + \boldsymbol{q}$ where $\boldsymbol{p}$ and $\boldsymbol{q}$ are two dimentional vectors. Also, after performing the contour integration over t_1 and t_2 and then evaluating the time integral in J, we are left with the expression

$$J = 4\int e^{iP\,p} A^{-i\alpha_B - 1}(A - B)^{i\alpha_B} C^{-i\alpha_A - 1}(C - D)^{i\alpha_A} d\boldsymbol{p}.$$

Finding J, J_1 and J_2 can be obtained from eq. (4) and so using eq. (3), the double differential cross section can be evaluated from eq. (2).

3. Results and discussions

Applying the above theoretical model, we have calculated the double differential cross sections for proton impact ionization of $3p$-electrons of Ar. It has now been established both by calculations [8–10] and measurements [11–14] of various targets that outer shell ionization gives the dominant contribution. We have therefore, compared our results of $3p$ ionization with the total (from all shells) differential cross sections of other theoretical as well as measurements. In Figure 1, we present our double differential cross sections along with the measurement of Rudd *et al* [5] and theoretical results of Fainstein *et al* [6] as a function of the ejection angle of the outgoing electron. The projectile velocity considered was 350 keV and at three electron velocities : (a) 46 eV, (b) 100 eV and (c) 308 eV. In all three figures, the solid curve represents present results. The short and long dash are the CDW-EIS and plane Born results of Fainstein *et al* [6] respectively. The plane Born results were calculated following Madison and Manson [15] but with a screened hydrogen-like wave function. The CDW-EIS results of Fainstein *et al* [6] give the best agreement with the measurements. However, it is interesting to note that measurements below 20° or above 150° are not available. It is these angular ranges where the present results differ with CDW-EIS results significantly. While below 20°, present results underestimate CDW-EIS results, they overestimate the CDW-EIS results above 150°. Nevertheless, the difference between the two calculations is reduced at 308 eV outgoing electron except at higher angles (Figure 1(c)). Similar trend is also noted for their plane Born results with screened hydrogen-like wave functions. The final state wave function in the present model differs with that of CDW-EIS model only in the choice of the centre of the reference frame, which should be invariant under Galilean transformation. The difference in the initial state wave function should have minimum effect at the impact energy considered here. However, the choice of interaction potential in the two calculations and the associated target wave function is perhaps responsible for the difference in results of two models. Fainstein *et al* [6] considered the interaction between the active electron and the passive electrons averaged over the passive electron wave function. The interaction in the present model, on the other hand, contains a long-range part to account the Coulomb interaction between the active electron and the target core and a short-range part to account the distortion, the correlation and indeed other effects of the passive electrons. The accuracy of the wave function was also tested by the virial theorem to within 0.01%.

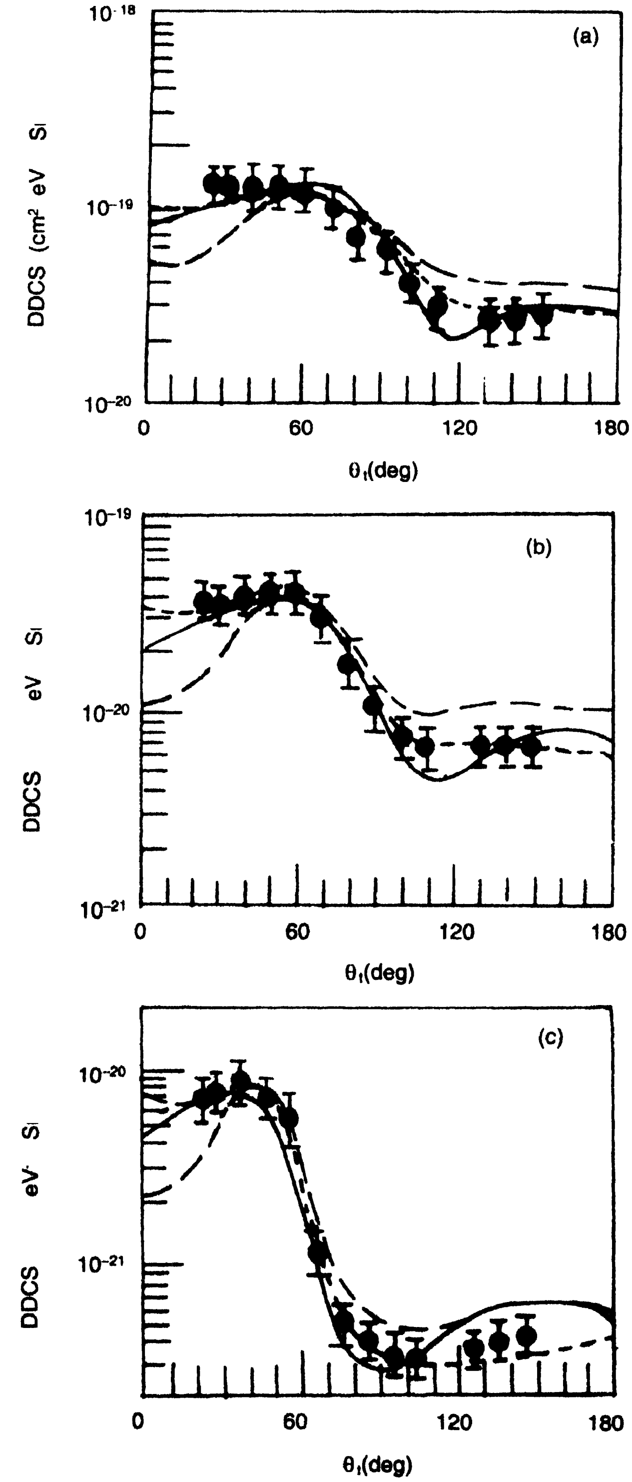

Figure 1. Double differential cross sections for electron emission at electron energies : (a) 46 eV, (b) 100 eV and (c) 308 eV. Incident proton velocity was taken to be 350 keV. The solid curve : present results, short dash : CDW-EIS results of Fainstein *et al* [6] and long dash : plane wave Born results of Fainstein *et al* [6] using the method of Madison and Manson [15]. Experiment : Rudd *et al* [5].

Acknowledgments

The authors are thankful to Professor N C Sil for many fruitful discussions. NCD acknowledges the financial support through the DST Grant No. SP/S2/L-12/99.

References

[1] G B Crooks M E Rudd *Phys. Rev. Lett.* **25** 1599 (1970)

[2] L Sarkadi, U Brinkman, A Báder, R Hippler, K Tökési and L Gulyás *Phys. Rev.* **A58** 296 (1998)

[3] M B Shah, C McGrath, C Illescas, B Pons, A Riera, H Luna, D S F Crothers, S F C O'Rourke and H B Gilbody *Phys. Rev.* **A67** 010704(R) (2003)

[4] L Sarkadi, J Bossler, R Hippler and O D Lutz *J. Phys.* **B16** 71 (1983)

[5] M E Rudd, L H Toburen and N Stolterfoht *At. Data Nucl. Data Tables* **23** 405 (1979)

[6] P D Fainstein, L Gulyás and S A Salin *J. Phys.* **B27** L259 (1994)

[7] L Gulyás, P D Fainstein and S A Salin *J. Phys.* **B28** 245 (1995)

[8] D S F Crothers and J F McCann *J. Phys.* **B16** 3229 (1983)

[9] S Bhattacharya, R Das, N C Deb, K Roy and D S F Crothers *Phys. Rev.* A68 052702 (2003)

[10] P D Fainstein and R D Rivarola *Phys. Lett.* **A150** 23 (1990)

[11] M Eckhardt and K H Schartner *Z. Phys.* **A312** 321 (1983)

[12] M E Rudd, Y K Kim, D H Madison and J W Gallaghar *Rev. Mod. Phys.* **57** (1985)

[13] C L Cocke, R K Gardner, B Curnutte, T Bratton and T K Saylor *Phys. Rev.* **A16** 2248 (1977)

[14] M Rødbro, E Horsdal Pedersen, C L Cocke and J R Macdonald *Phys. Rev.* **A19** 1936 (1979)

[15] D H Madison and S T Manson *Phys. Rev.* **A20** 825 (1979)